Black Box Variational Bayes with a Deterministic Objective

Faster, More Accurate, and Even More Black Box

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May 25th, 2023

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Problem statement

We all want to do accurate Bayesian inference quickly:

- In terms of compute (wall time, model evaluations, parallelism)
- In terms of analyst effort (tuning, algorithmic complexity)

Markov Chain Monte Carlo (MCMC) can be straightforward and accurate but slow.

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Markov Chain Monte Carlo (MCMC) can be straightforward and accurate but slow.

Black Box Variational Inference (BBVI) can be faster alternative to MCMC. **But...**

- BBVI is cast as an optimization problem with an intractable objective $\Rightarrow$
- Most BBVI methods use **stochastic gradient** (SG) optimization $\Rightarrow$
  - SG algorithms can be hard to tune
  - Assessing convergence and stochastic error can be difficult
  - SG optimization can perform worse than second-order methods on tractable objectives
- Many BBVI methods employ a **mean-field (MF) approximation** $\Rightarrow$
  - Posterior variances are poorly estimated

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Our proposal: replace the intractable BBVI objective with a fixed approximation.

- Better optimization methods can be used (e.g. true second-order methods)
- Convergence and approximation error can be assessed directly
- Can correct posterior covariances with linear response covariances
- This technique is well-studied (but there's still work to do in the context of BBVI)

$\Rightarrow$ **Simpler, faster, and better BBVI posterior approximations ... in some cases.**

Outline

- BBVI Background and our proposal
  - Automatic differentiation variational inference (ADVI) (a BBVI method)
  - Our approximation: "Deterministic ADVI" (DADVI)
  - Linear response (LR) covariances
  - Estimating approximation error
- Experimental results: DADVI vs ADVI
  - DADVI converges faster than ADVI, and requires no tuning
  - DADVI's posterior mean estimates' accuracy are comparable to ADVI
  - DADVI+LR provides more accurate posterior variance estimates than ADVI
  - DADVI provides accurate estimates of its own approximation error
  - But stochastic ADVI often results in better objective function values (eventually)
- Theory and shortcomings
  - Pessimistic dimension dependence results from optimization theory
  - ...which do not apply in certain BBVI settings.
  - DADVI fails for expressive BBVI approximations (e.g. full-rank ADVI)
  - More work to be done!

Notation

Parameter:	$\theta \in \mathbb{R}^{D_\theta}$
Data:	y
Prior:	$\mathcal{P}(\theta)$ (density w.r.t. Lebesgue $\mathbb{R}^{D_\theta}$, nonzero everywhere)
Likelihood:	$\mathcal{P}(y\|\theta)$ (nonzero for all θ)

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$$\mathcal{P}(\theta|y) = \frac{\mathcal{P}(\theta, y)}{\int \mathcal{P}(\theta', y) d\theta'}.$$

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Denote gradients with ∇, e.g.,

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Assume we have a twice auto-differentiable software implementation of

$$\theta \mapsto \log \mathcal{P}(\theta, y) = \log \mathcal{P}(y|\theta) + \log \mathcal{P}(\theta).$$

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We will study **ADVI**, a particular BBVI method [Kucukelbir et al., 2017].

ADVI specifies a family $\Omega_{\mathcal{Q}}$ of D_θ-dimensional Gaussian distributions, parameterized by $\eta \in \mathbb{R}^{D_\eta}$, encoding the means and covariances. The covariances can either be

- Diagonal: "Mean-field" (MF) approximation, $D_\eta = 2D_\theta$
- Any PD matrix: "Full-rank" (FR) approximation, $D_\eta = D_\theta + D_\theta(D_\theta - 1)/2$

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$$\underset{\mathcal{Q}\in\Omega_{\mathcal{Q}}}{\operatorname{argmin}} \operatorname{KL}\left(\mathcal{Q}(\theta|\eta)||\mathcal{P}(\theta|y)\right) = \underset{\eta\in\mathbb{R}^{D_\eta}}{\operatorname{argmin}} \operatorname{KL}_{\mathrm{VI}}(\eta) \quad \text{where}$$

$$\operatorname{KL}_{\mathrm{VI}}(\eta) := \underbrace{\mathop{\mathbb{E}}_{\mathcal{N}_{\mathrm{std}}(z)}\left[\log \mathcal{Q}(\theta(z,\eta)|\eta)\right]}_{\text{Available in closed form}} - \underbrace{\mathop{\mathbb{E}}_{\mathcal{N}_{\mathrm{std}}(z)}\left[\log \mathcal{P}(\theta(z,\eta),y)\right]}_{\text{Typically intractable}}.$$

The final line uses the "reparameterization trick" with standard Gaussian $z \sim \mathcal{N}_{\mathrm{std}}(z)$.

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ADVI is an instance of the *general problem* of finding

$$\operatorname*{argmin}_{\eta} F(\eta) \quad \text{where} \quad F(\eta) := \mathop{\mathbb{E}}_{\mathcal{N}_{\mathrm{std}}(z)}\left[f(\eta,z)\right].$$

Two approaches

$$\text{Consider} \quad \operatorname*{argmin}_{\eta} F(\eta) \quad \text{where} \quad F(\eta) := \mathop{\mathbb{E}}_{\mathcal{N}_{\mathrm{std}}(z)} \left[f(\eta, z) \right].$$

Let $\mathcal{Z}_N = \{z_1, \ldots, z_N\} \overset{iid}{\sim} \mathcal{N}_{\mathrm{std}}(z)$, and let $\hat{F}(\eta | \mathcal{Z}_N) := \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n)$.

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Algorithm 1
Stochastic gradient (SG)
ADVI (and most BBVI)

Fix N (typically $N = 1$)
$t \leftarrow 0$
while Not converged **do**
  $t \leftarrow t + 1$
  Draw $\mathcal{Z}_N$
  $\Delta_S \leftarrow \nabla_\eta \hat{F}(\eta_{t-1} | \mathcal{Z}_N)$
  $\alpha_t \leftarrow \mathrm{SetStepSize}(\text{Past state})$
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Algorithm 2
Sample average approximation (SAA)
Deterministic ADVI (DADVI) (proposal)

Fix N (our experiments use $N = 30$)
Draw $\mathcal{Z}_N$
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while Not converged **do**
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Our proposal: Apply Algorithm 2 with the ADVI objective.
Take better steps, easily assess convergence, with less tuning.

Experiments

For each of a range of models (next slide), we compared:

- **NUTS:** The "no-U-turn" MCMC sampler as implemented by PyMC [Salvatier et al., 2016]. We used this as the "ground truth" posterior.

- **DADVI:** We used $N = 30$ draws for DADVI for each model. We optimized using an off-the-shelf second-order Newton trust region method (`trust-ncg` in `scipy.optimize.minimize`) with no tuning or preconditioning.

Stochastic ADVI methods:

- Mean field ADVI: We used the PyMC implementation of ADVI, together with its default termination criterion (based on parameter differences).
- Full-rank ADVI: We used the PyMC implementation of full-rank ADVI, together with the default termination criterion for ADVI described above.
- RAABBVI: To run RAABBVI, we used the public package `viabel`, provided by Welandawe et al. [2022].

We terminated unconverged stochastic ADVI after 100,000 iterations.

Experiments

We evaluated each method on a range of models.

Model Name	Dim D_θ	NUTS runtime	Description
ARM (53 models)	Median 5 (max 176)	median 39 seconds (max 16 minutes)	A range of linear models, GLMs, and GLMMs
Microcredit	124	597 minutes	Hierarchical model with heavy tails and zero inflation
Occupancy	$1,884$	251 minutes	Binary regression with highly crossed random effects
Tennis	$5,014$	57 minutes	Binary regression with highly crossed random effects
POTUS	$15,098$	643 minutes	Autoregressive time series with random effects

Table 1: Model summaries.

Comparisons

To form a common scale for the accuracy of the posteriors, we report:

$$\varepsilon^{\mu}_{\text{METHOD}} := \frac{\mu_{\text{METHOD}} - \mu_{\text{NUTS}}}{\sigma_{\text{NUTS}}} \qquad \varepsilon^{\sigma}_{\text{METHOD}} := \frac{\sigma_{\text{METHOD}} - \sigma_{\text{NUTS}}}{\sigma_{\text{NUTS}}}.$$

where

$$\mu_{\text{METHOD}} := \text{METHOD posterior mean} \qquad \sigma_{\text{METHOD}} := \text{METHOD posterior SD}.$$

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We measure computational cost using both

- **Wall time** and
- **Number of model evaluations** (gradients, Hessian-vector products).

We compare achieved objective values using a large number of independent samples.

We report objective values and computation cost relative to DADVI.

Posterior mean accuracy

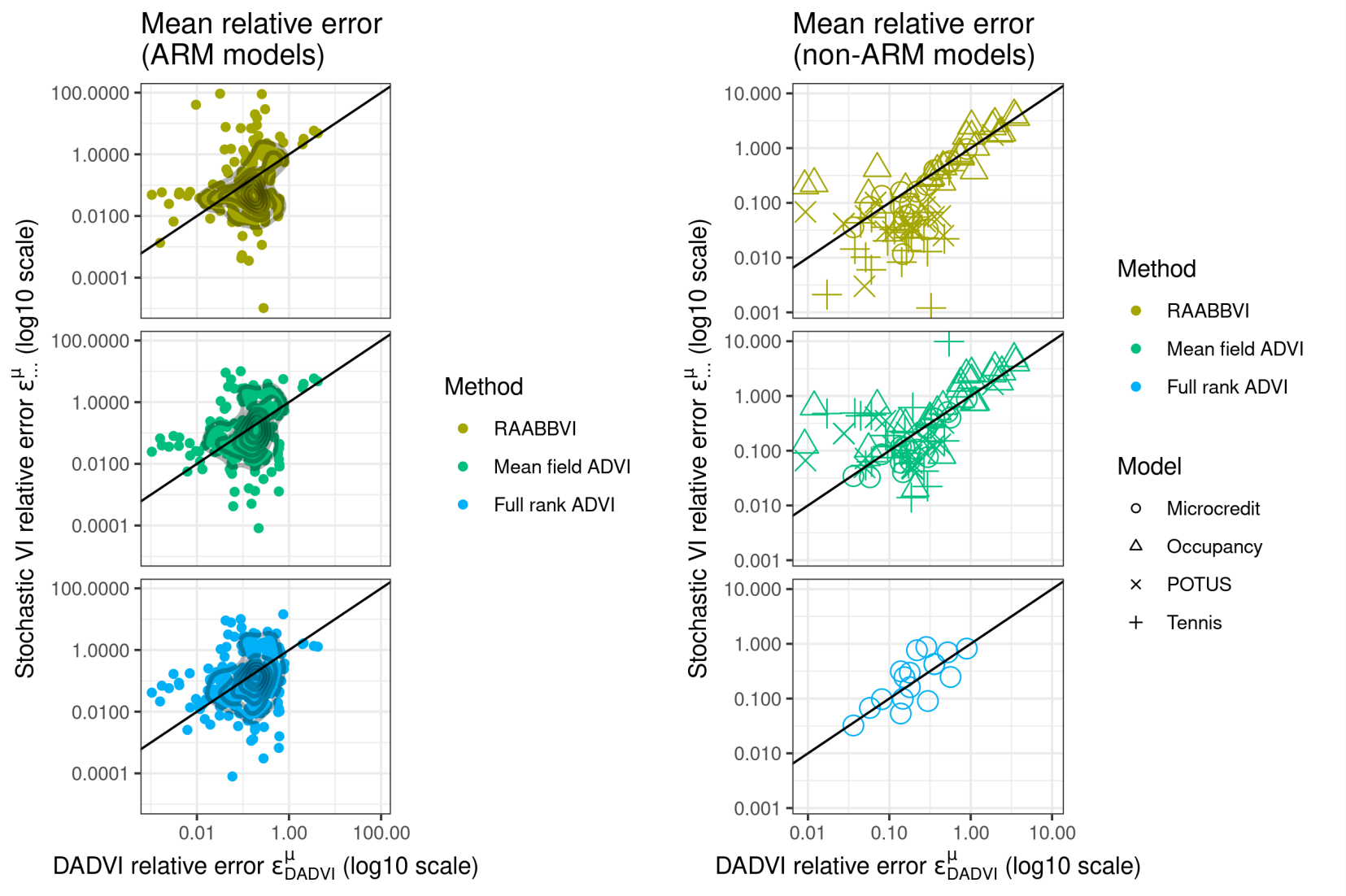


Figure 1: Posterior mean accuracy (relative to MCMC posterior standard deviation). Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.

Computational cost for ARM models

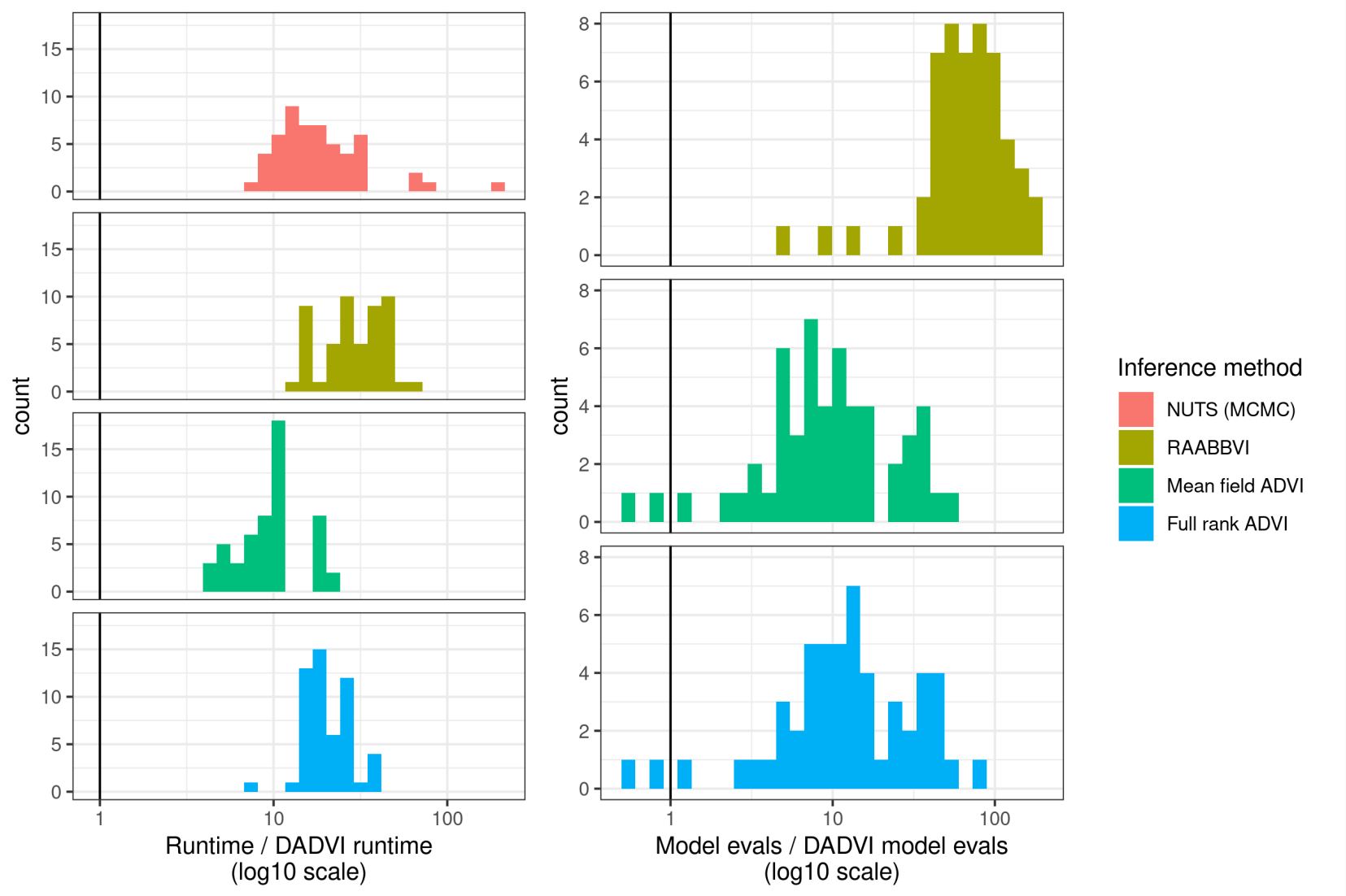


Figure 2: Runtimes and model evaluation counts for the ARM models. Results are reported divided by the corresponding value for DADVI.

Computational cost for non-ARM models

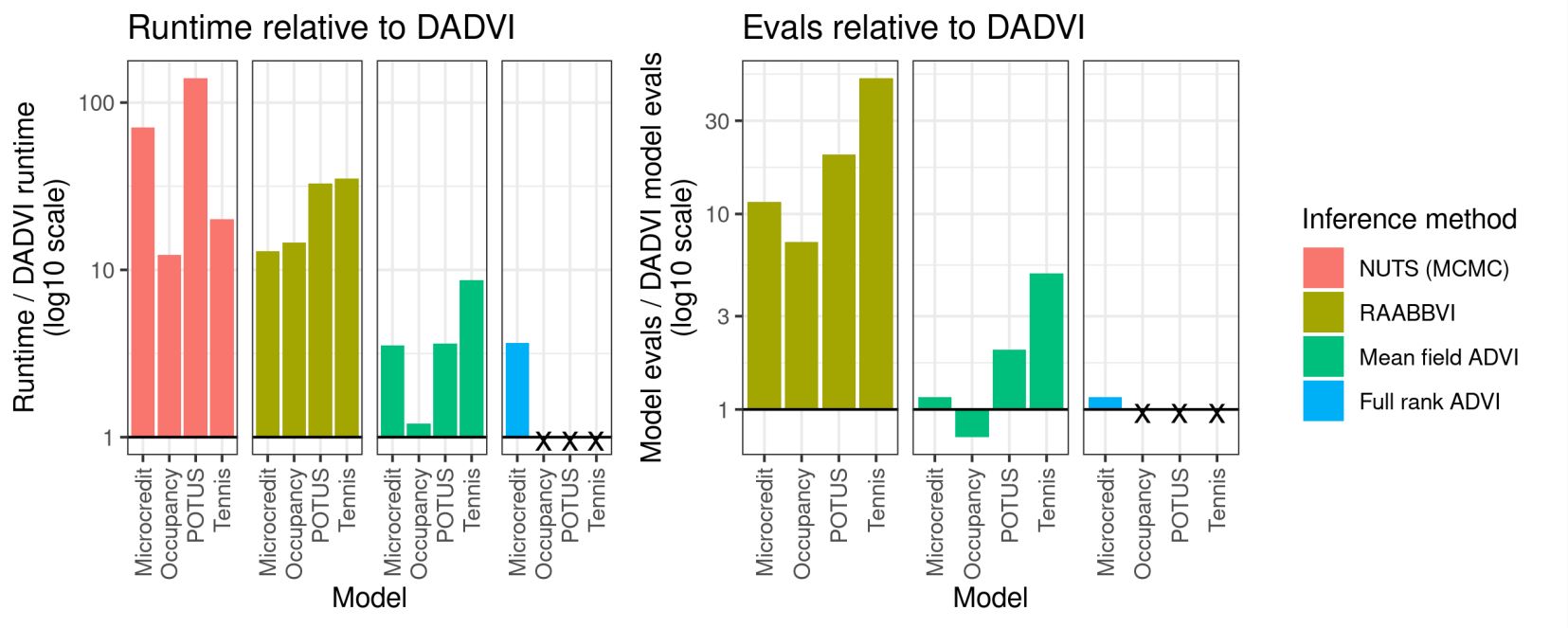


Figure 3: Runtimes and model evaluation counts for the non-ARM models. Results are reported divided by the corresponding value for DADVI. Missing model / method combinations are marked with an X.

Optimization traces for ARM models

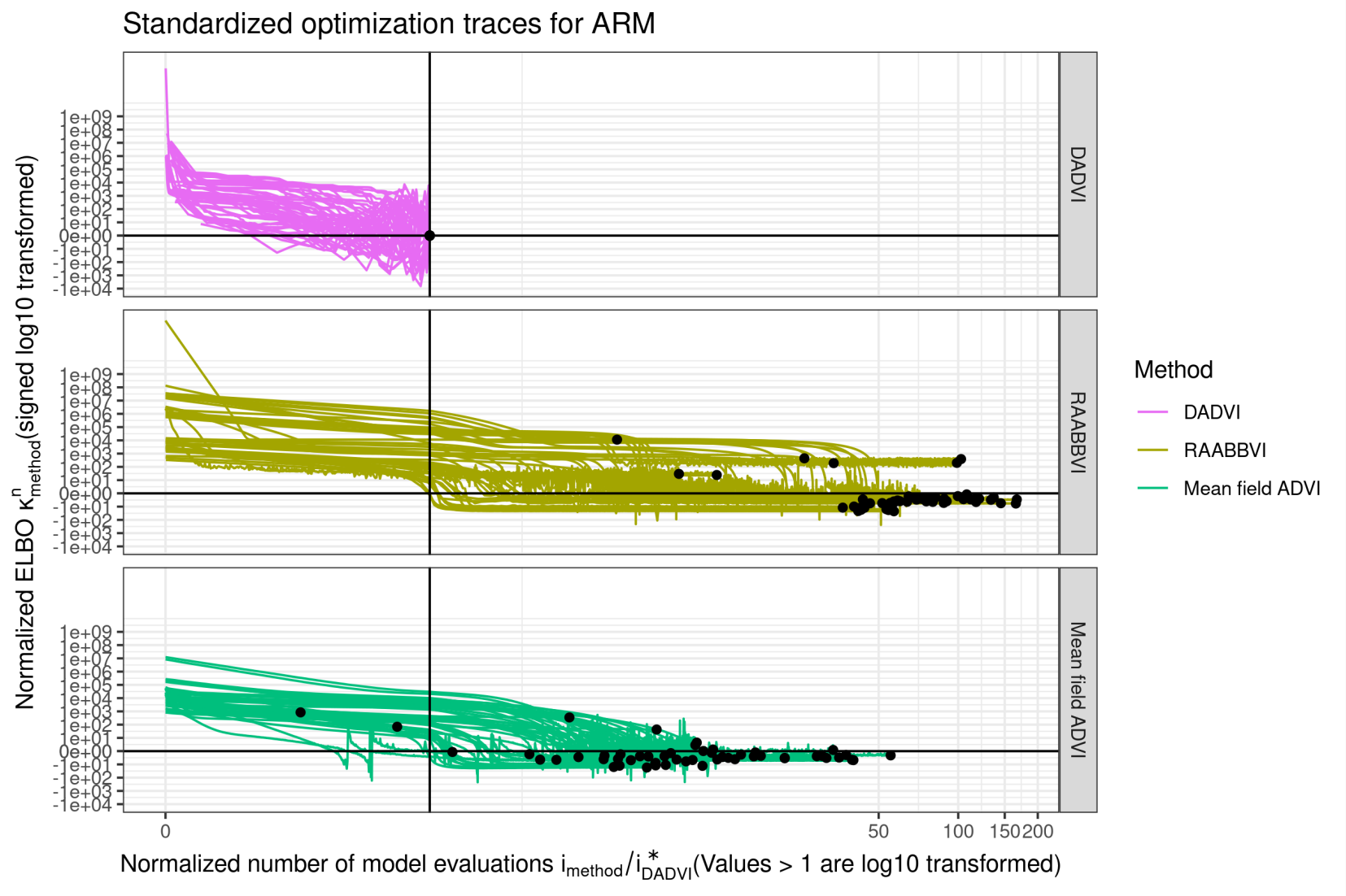
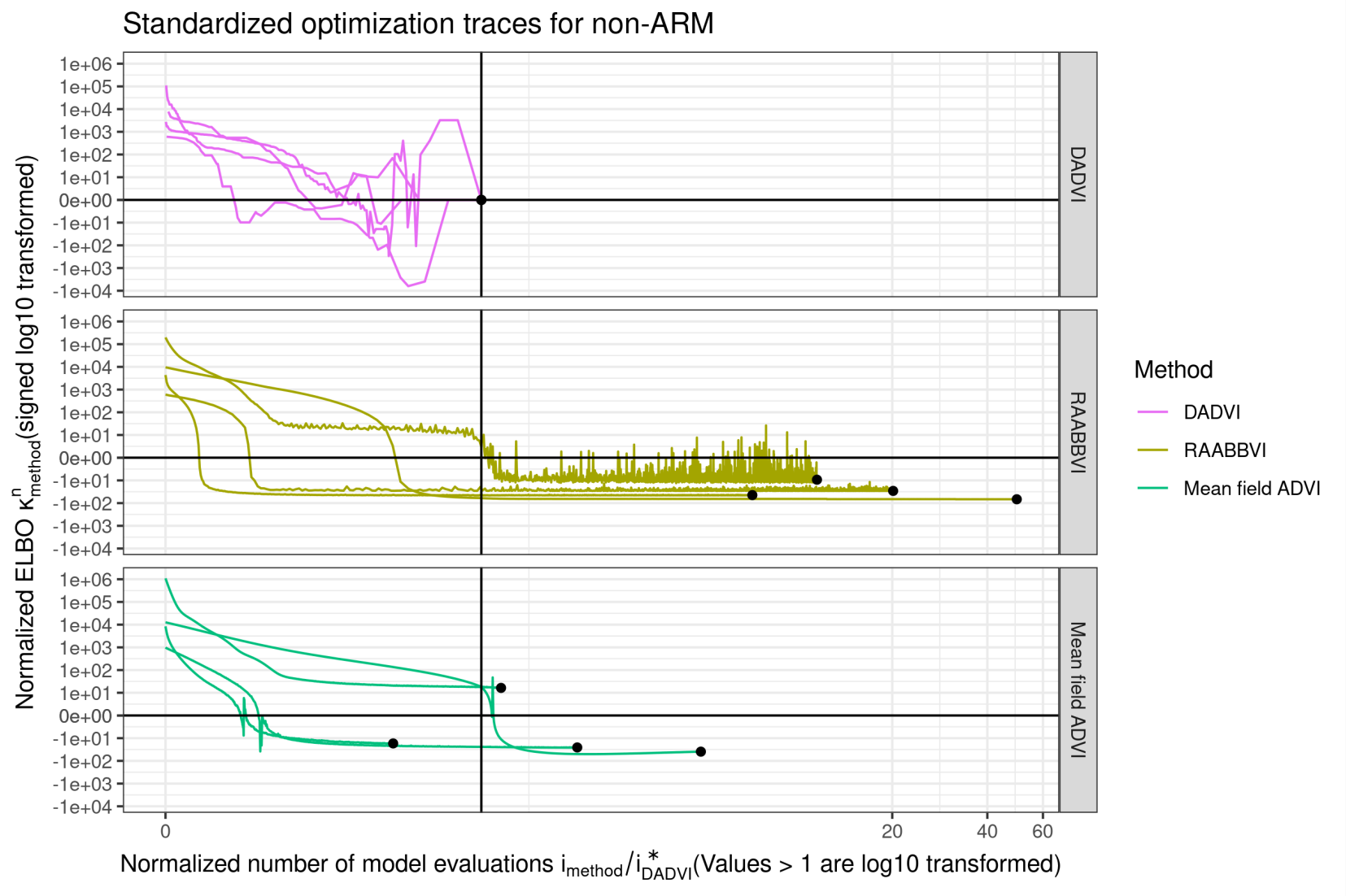


Figure 4: Optimization traces for the ARM models. Black dots show the termination point of each method. Dots above the horizontal black line mean that DADVI found a better ELBO. Dots to the right of the black line mean that DADVI terminated sooner in terms of model evaluations.

Optimization traces for non-ARM models



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Experiment summary

$\Rightarrow$ DADVI is faster, simpler, and the posterior means are not worse.

But DADVI can additionally provide:

- Simple estimates of approximation error
- Improved (LR) posterior covariance esimates

Linear response covariances and sampling uncertainty

Intractable objective:

$$\overset{*}{\eta} = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$$

DADVI approximation:

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What is the error of the DADVI approximation $\hat{\eta} - \overset{*}{\eta}$?

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Answer: The same as a that of any M-estimator: asymptotically normal (as N grows)

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Posterior variances are often badly estimated by mean-field (MF) approximations.

Linear response (LR) covariances improve covariance estimates by computing *sensitivity* of the variational means to particular perturbations. [Giordano et al., 2018]

Example: With a correlated Gaussian $\mathcal{P}(\theta|y)$, the ADVI means are exactly correct, the ADVI variances are underestimated, and LR covariances are exactly correct.

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Both DADVI error and LR covariances can be computed from the DADVI objective.

Stochastic ADVI does not produce an actual optimum of any tractable objective, so LR and M-estimator computations are unavailable.

Posterior standard deviation accuracy

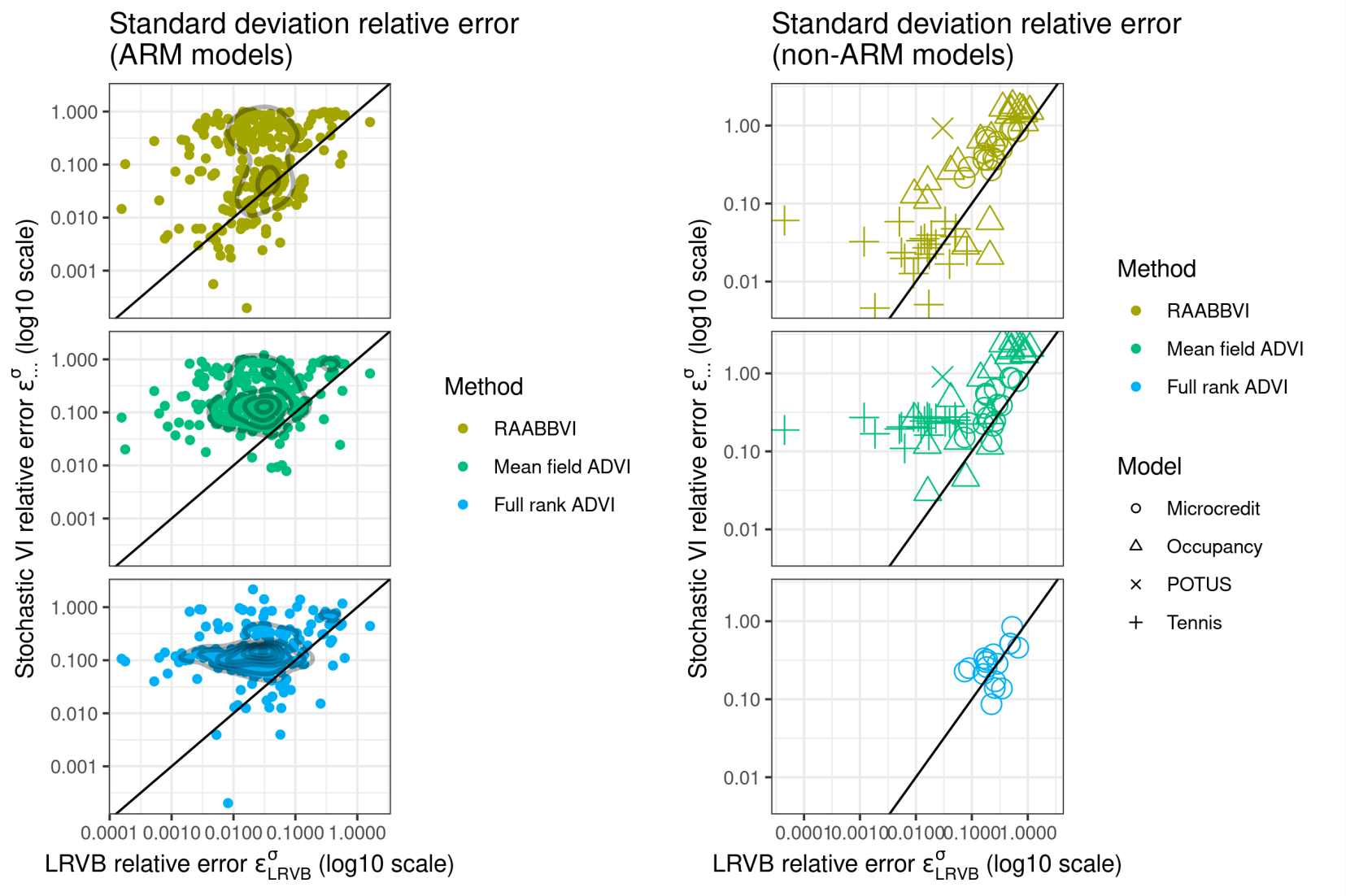

Figure 6: Posterior sd relative accuracy. Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.

DADVI approximation error accuracy

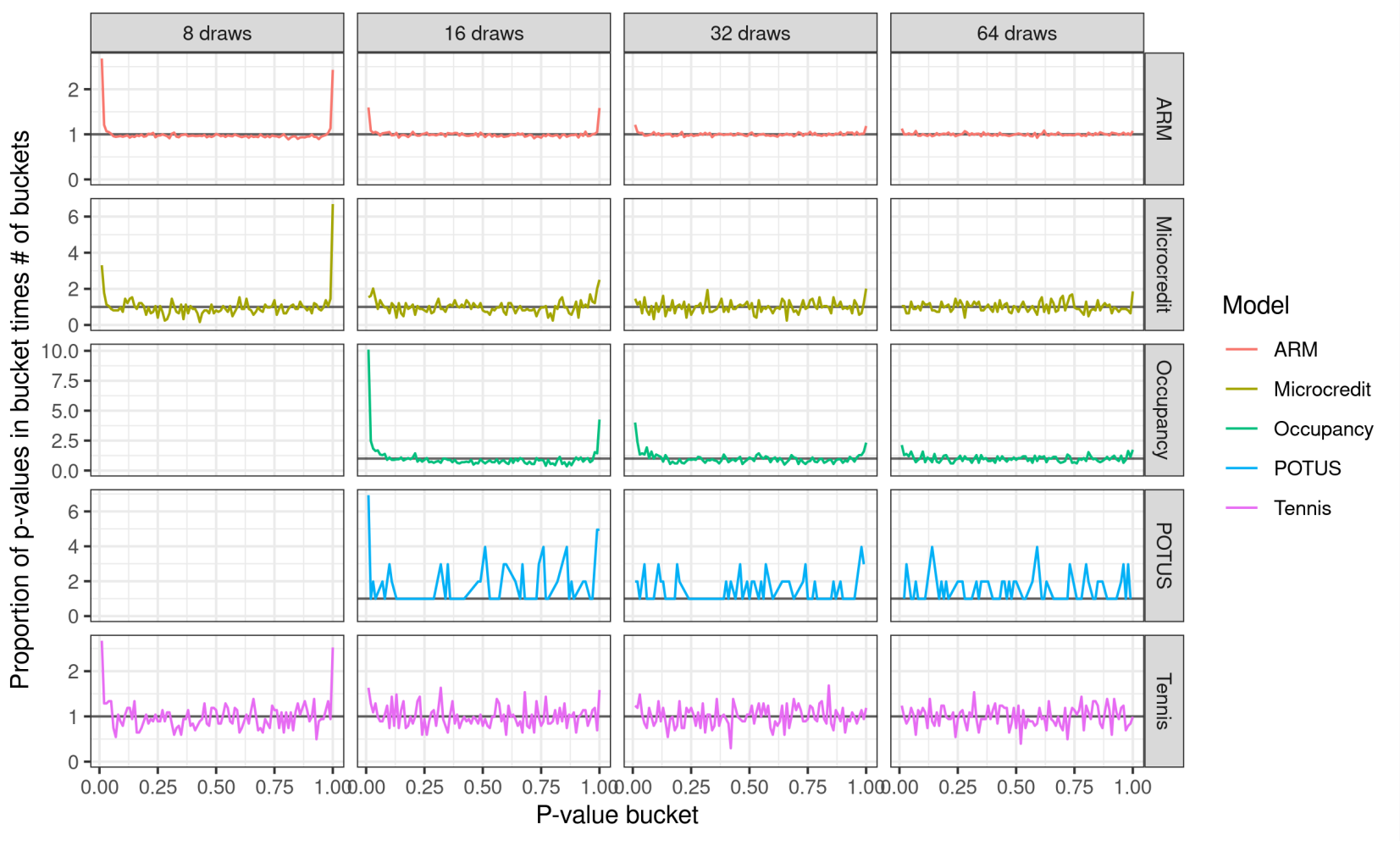

Figure 7: Density estimates of $\Phi(\varepsilon^{\xi})$ for difference models. All the ARM models are grouped together for ease of visualization. Each panel shows a binned estimate of the density of $\Phi(\varepsilon^{\xi})$ for a particular model and number of draws N. Values close to one (a uniform density) indicate good frequentist performance. CG failed for the Occupancy and POTUS models with only 8 draws, possibly indicating poor optimization performance with so few samples.

Previous theoretical results

Intractable objective:

$$\overset{*}{\eta} = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$$

SAA approximation (DADVI):

$$\hat{\eta}(\mathcal{Z}_N) = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n).$$

The idea of optimizing $\hat{F}$ instead of SG on F is old and well-studied in the optimization literature, where $\hat{F}$ is known as the **Sample average approximation (SAA)**.

Yet SAA is rarely used for BBVI.[1] One possible reason is the following:

Theorem [Nemirovski et al., 2009]: In general, the error of both SG and SAA scale as $\sqrt{D_\theta / N}$, where, for SG, N is the *total number of samples used*.

[1] Some exceptions I'm aware of: Giordano et al. [2018, 2022], Wycoff et al. [2022], Burroni et al. [2023].

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$$\hat{\eta}(\mathcal{Z}_N) = \underset{\eta \in \mathbb{R}^{D_\eta}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n).$$

The idea of optimizing $\hat{F}$ instead of SG on F is old and well-studied in the optimization literature, where $\hat{F}$ is known as the **Sample average approximation (SAA)**.

Yet SAA is rarely used for BBVI.[1] One possible reason is the following:

Theorem [Nemirovski et al., 2009]: In general, the error of both SG and SAA scale as $\sqrt{D_\theta / N}$, where, for SG, N is the *total number of samples used*.

- For SG, each z_n gets used once (for a single gradient step)
- For SAA, each z_n gets used once per optimization step (of which the are many).
- Often, in higher dimensions, SAA requires more optimization steps.

Corollary: [Kim et al., 2015] In general, for a given accuracy, the computation required for SAA scales worse than SG as the dimension D_θ grows.

[1] Some exceptions I'm aware of: Giordano et al. [2018, 2022], Wycoff et al. [2022], Burroni et al. [2023].

Previous theoretical results

Intractable objective:

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But we got good results with D_θ as high as $15,098$ using only only $N = 30$. Why?

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Some first steps

Theorem [Giordano et al., 2023]: When $\mathcal{P}(\theta|y)$ is multivariate normal, and we use the mean-field Gaussian approximation, then, for any particular entry η_d of η, then $\left|\hat{\eta}_d - \overset{*}{\eta}_d\right| = O_p(N^{-1/2})$ irrespective of D_θ.

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Theorem [Giordano et al., 2023]: Assume $\mathcal{P}(\theta|y)$ has a "global-local" structure:

$$\theta = (\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}) \qquad \mathcal{P}(\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}|y) = \prod_{d=1}^{D_\lambda} \mathcal{P}(\gamma, \lambda_d|y).$$

Assume that the dimension of γ and each λ_d stays fixed as D_λ grows.

Under regularity conditions, the DADVI error scales as $\sqrt{\log D_\lambda / N}$, not $\sqrt{D_\lambda / N}$.

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Under regularity conditions, the DADVI error scales as $\sqrt{\log D_\lambda / N}$, not $\sqrt{D_\lambda / N}$.

Proposal: The "in general" analysis of [Nemirovski et al., 2009] is too general for many practically interesting BBVI problems.

A negative result for expressive approximations

Theorem [Giordano et al., 2023]: Assume that $N < D_\theta$, and that we use a full-rank Gaussian approximation. Then the DADVI objective is unbounded below, and optimization of the DADVI objective will approach a degenerate point mass at $\mathrm{argmax}_\theta \log \mathcal{P}(\theta|y)$.

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Proof sketch: For any value of the variational mean, the DADVI objective only depends on $\mathcal{P}(\theta|y)$ evaluated in a subspace spanned by $\mathcal{Z}_N$. The variational objective can be driven to $-\infty$ by driving the variance to zero in the subspace orthogonal to $\mathcal{Z}_N$.

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Proposal: All sufficiently expressive variational approximations (e.g. normalizing flows) will fail in the same way in high dimensions. However, this pathology can be obscured and overlooked in practice by low-quality optimization.

Conclusion

Black Box Variational Inference with a Deterministic Objective: Faster, More Accurate, and Even More Black Box.

Giordano, R.*, Ingram, M.*, Broderick, T. (* joint first authors), 2023.

(Arxiv preprint here.)

- By fixing the randomness in the ADVI objective, DADVI provides BBVI that is easier to use, faster, and more accurate than stochastic gradient.
- The approximation used by DADVI will not work in high dimensions for sufficiently expressive approximating distributions (e.g., full-rank ADVI).
- There appears to be a gap between the optimization literature and BBVI practice in high dimensions for a class of practically interesting problems.

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Supplemental material

Linear response covariances

Posterior variances are often badly estimated by mean-field (MF) approximations.

Example: With a correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI, the ADVI means are correct, but the ADVI variances are underestimated.

Take a variational approximation $\overset{*}{\eta} := \operatorname{argmin}_{\eta \in \mathbb{R}^{D_\eta}} \mathrm{KL}_{\mathrm{VI}}(\eta)$. Often,

$$\mathop{\mathbb{E}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}[\theta] \approx \mathop{\mathbb{E}}_{\mathcal{P}(\theta|y)}[\theta] \quad \text{but} \quad \mathop{\mathrm{Var}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}(\theta) \neq \mathop{\mathrm{Var}}_{\mathcal{P}(\theta|y)}(\theta)\,. \tag{1}$$

Example: Correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI.

Linear response covariances use the fact that, if $\mathcal{P}(\theta|y,t) \propto \mathcal{P}(\theta|y)\exp(t\theta)$, then

$$\left.\frac{d \mathop{\mathbb{E}}_{\mathcal{P}(\theta|y,t)}[\theta]}{dt}\right|_{t=0} = \mathop{\mathrm{Cov}}_{\mathcal{P}(\theta|y)}(\theta)\,. \tag{2}$$

Let $\overset{*}{\eta}(t)$ be the variational approximation to $\mathcal{P}(\theta|y,t)$, and take

$$\mathop{\mathrm{LRCov}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}(\theta) = \left.\frac{d \mathop{\mathbb{E}}_{\mathcal{Q}(\theta|\overset{*}{\eta}(t))}[\theta]}{dt}\right|_{t=0} = \left(\nabla_\eta \mathop{\mathbb{E}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}[\theta]\right)\left(\nabla^2_\eta \mathrm{KL}_{\mathrm{VI}}(\overset{*}{\eta})\right)^{-1}\left(\nabla_\eta \mathop{\mathbb{E}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}[\theta]\right)$$

Example: For ADVI with a correlated Gaussian $\mathcal{P}(\theta|y)$, $\mathop{\mathrm{LRCov}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}(\theta) = \mathop{\mathrm{Cov}}_{\mathcal{Q}(\theta|\overset{*}{\eta})}(\theta)$.